



Bioaccumulation Model Calibration Update

CPG-EPA Meeting

July 12, 2018

Agenda

- Review action items from June meeting
- Parameter distribution review for select parameters
 - Metabolic rate distributions
 - E_D value distributions
- Calibration update
 - Three calibration options
 - Steady state and dynamic model results
- Next Steps



REVIEW OF DISTRIBUTIONS

Preliminary E_D Distributions

Distributions pending additional research, which is ongoing.

Chemical	Nominal Value	Range	Rationale
2,3,7,8-TCDD	0.37	0.004 – 0.48 <i>(literature: 0.12 – 0.45)</i>	<u>Nominal</u> : calculated based on K _{OW} of 6.38. <u>Range</u> : Includes range of calculated values based K _{OW} (5.38-8.93) and literature values.
TetraCB	0.45	0.30 – 0.48	<u>Nominal</u> : calculated based on K _{OW} of 5.85. <u>Range</u> : Includes range of calculated values based K _{OW} (5.38-6.65).
1,2,3,4,6,7,8-HpCDF	0.03	0.002 – 0.11	<u>Nominal</u> : calculated based on K _{OW} of 8.03. <u>Range</u> : Includes range of calculated values based K _{OW} (7.37-9.25).

Metabolic Rate Distribution

- Re-evaluated since this is a key parameter
- Based on Arnot et al. 2008
- Looked at different options for normalizing to weights of modeled species and options for grouping of species.

K_M for 2378-TCDD

Species Group	Nominal Value	Range	Rationale
Benthic inverts	0.013	0.002 – 0.082	No information, so used same distribution as for small fish.
Small fish	0.013	0.002 – 0.082	<u>Nominal</u> : Average of values normalized for 10 g fish. <u>Range</u> : 2.5 th to 97.5 th percentile for values normalized to 10 g fish.
Carp	0.003	0.0004 – 0.013	Carp-specific data available, so used these values normalized to weight of modeled carp. <u>Nominal</u> : average of values <u>Range</u> : 2.5 th to 97.5 th percentiles
Blue crab	0.006	0.0005 – 0.045	Calculated Km values based on weights for these FWM species. Same distribution used for these two groups, but calibrated value allowed to be different.
Eel	0.006	0.0005 – 0.045	<u>Nominal</u> : average of adjusted values <u>Range</u> : 2.5 th to 97.5 th percentile for adjusted values
Other fish	0.006	0.0005 – 0.045	

K_M for TetraCB

Species Group	Nominal Value	Range	Rationale
Inverts	0	na	
Other fish	0	na	No change; available information does not support use of metabolic rate for most species.
Blue crab	0.002	0.0004 – 0.014	Revised from previous range based on calculating of K _M values using average weight for eel and blue crab, using same approach as was done for the 2015 calibration report. <u>Nominal:</u> Weighted average based on percent contribution to sediment for congeners with available K _M values. <u>Range:</u> Weighted average for 2.5 and 97.5 percentiles.
Eel	0.002	0.0004 – 0.014	

K_M for 1234678-HpCDF

Species Group	Nominal Value	Range	Rationale
Benthic inverts	0.086	0.031 – 0.24	No information, so used same values as for small fish.
Small fish	0.086	0.031 – 0.24	<u>Nominal</u> : Average of values normalized for 10 g fish. <u>Range</u> : 2.5 th to 97.5 th percentile for values normalized to 10 g fish.
Carp	0.036	0.007 – 0.13	Calculated K_M values based on weights for other FWM species. Same distribution used for these three groups, but calibrated value allowed to be different.
Eel	0.036	0.007 – 0.13	<u>Nominal</u> : average of adjusted values <u>Range</u> : 2.5 th to 97.5 th percentile for adjusted values
Other fish	0.036	0.007 – 0.13	
Blue crab	0.036	0.007 – 0.13	

CALIBRATIONS (USING STEADY STATE MODEL)

Calibration Process

1. Evaluate uncalibrated model results
2. Perform initial calibration using specific set of parameters
3. Evaluate results and develop strategies for alternative calibrations

Initial Calibration

- Changed K_{OW} values to match CFT model
- Updated E_D values to more optimal numbers
- Other changes that were agreed upon in June:

Parameter	Nominal	Range	Select-ed	Selected Value Min-----(Nominal)-----Max
Weight of DEPs (RM 6-14.7)	36 mg	0.12-400 mg	1 mg	0.12  (36) 400
Invert dietary AE of NLOC/NLOM	0.75	0.15-0.96	0.4	0.15  (0.75) 0.9
Percent of sediment in DEP diet (RM 6-14.7 and 14.7-Dam)	89%	70-100%	70% (min)	70%  (89%) 100%
DO Saturation (RM 6-14.7)	85%	71-97%	80%	71%  (85%) 97%

Initial Calibration – SPAFs

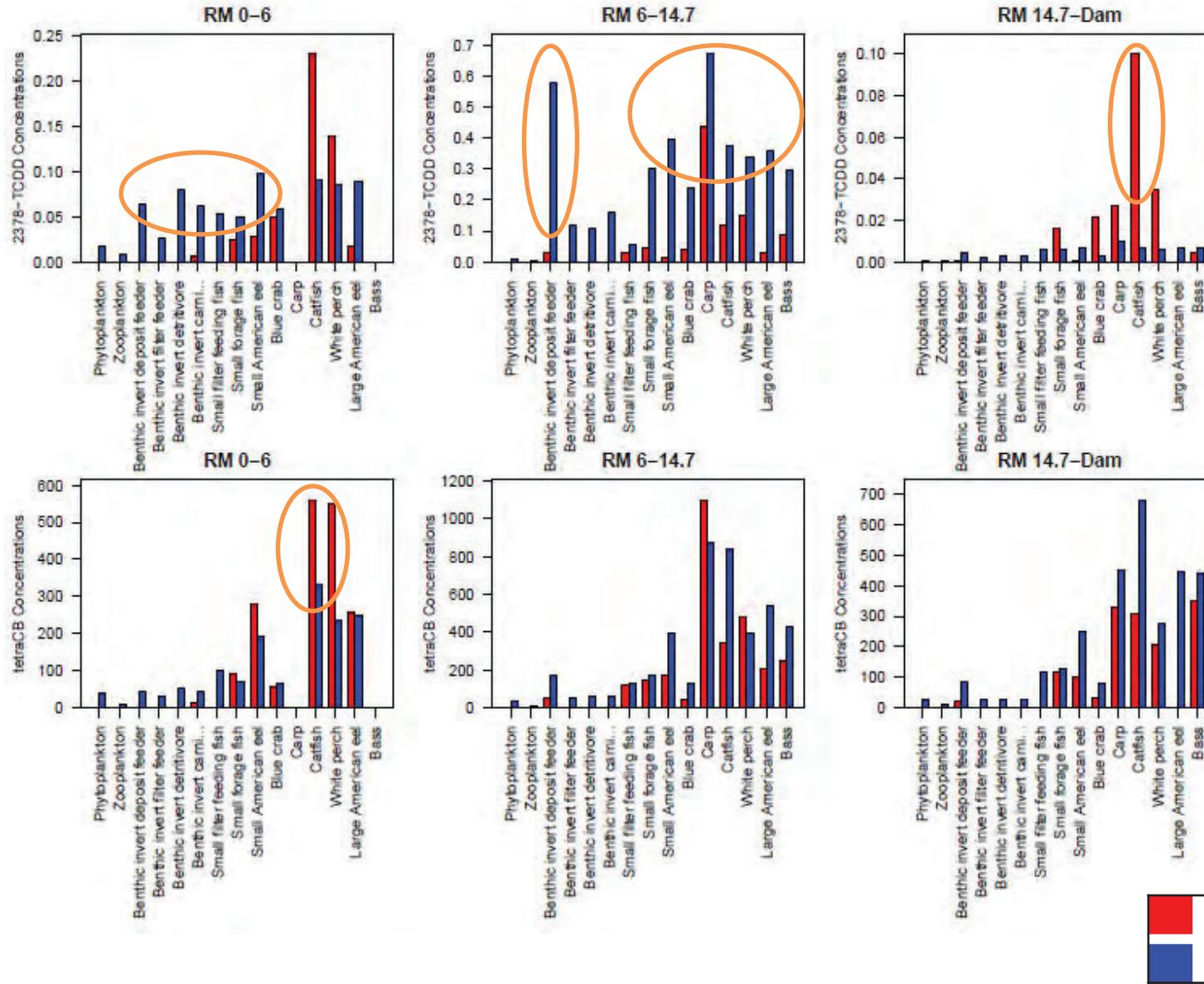
UNCALIBRATED

Species	2378-TCDD			TetraCB		
	RM 0-6	RM 6- 14.7	RM 14.7- Dam	RM 0-6	RM 6- 14.7	RM 14.7- Dam
DEP		50.8	10.4		6.2	3.7
FF						
DET						
C/O	14.1			2.5		
Small filter feeding fish		2.6			-1.1	
Small forage fish	3.2	17.3	-1.7	-1.6	1.3	-1.1
Small American eel	7.4	103.1	20.8	-1.7	3.1	2.2
Blue crab	2.3	17.8	-3.4	-1.0	3.9	2.3
Carp		3.2	-1.6		-1.2	1.3
Catfish	-1.3	10.3	-6.1	-2.0	2.8	1.8
White perch	1.3	7.9	-2.7	-2.9	1.0	1.1
Large American eel	11.7	43.3		-1.2	3.1	
Bass		13.5	4.2		1.9	-1.0
Average (all)	4.5	24.3	5.8	1.7	2.1	1.5
Average (priority)	22.0			2.2		

INITIAL CALIBRATION

	2378-TCDD			TetraCB		
	RM 0-6	RM 6- 14.7	RM 14.7- Dam	RM 0-6	RM 6- 14.7	RM 14.7- Dam
		20.0	9.0		3.1	4.0
	10.1			3.0		
		1.9			1.0	
	2.0	6.3	-2.8	-1.3	1.1	1.1
	3.5	30.6	9.9	-1.5	2.3	2.5
	1.2	5.7	-6.9	1.1	2.7	2.5
		1.5	-2.7		-1.3	1.4
	-2.6	3.1	-15.0	-1.7	2.5	2.2
	-1.6	2.3	-5.7	-2.3	-1.2	1.3
	5.2	11.6		-1.0	2.6	
		3.4	1.6		1.7	1.3
	2.7	7.4	6.4	1.5	1.8	1.7
	6.7			1.9		

Initial Calibration Results

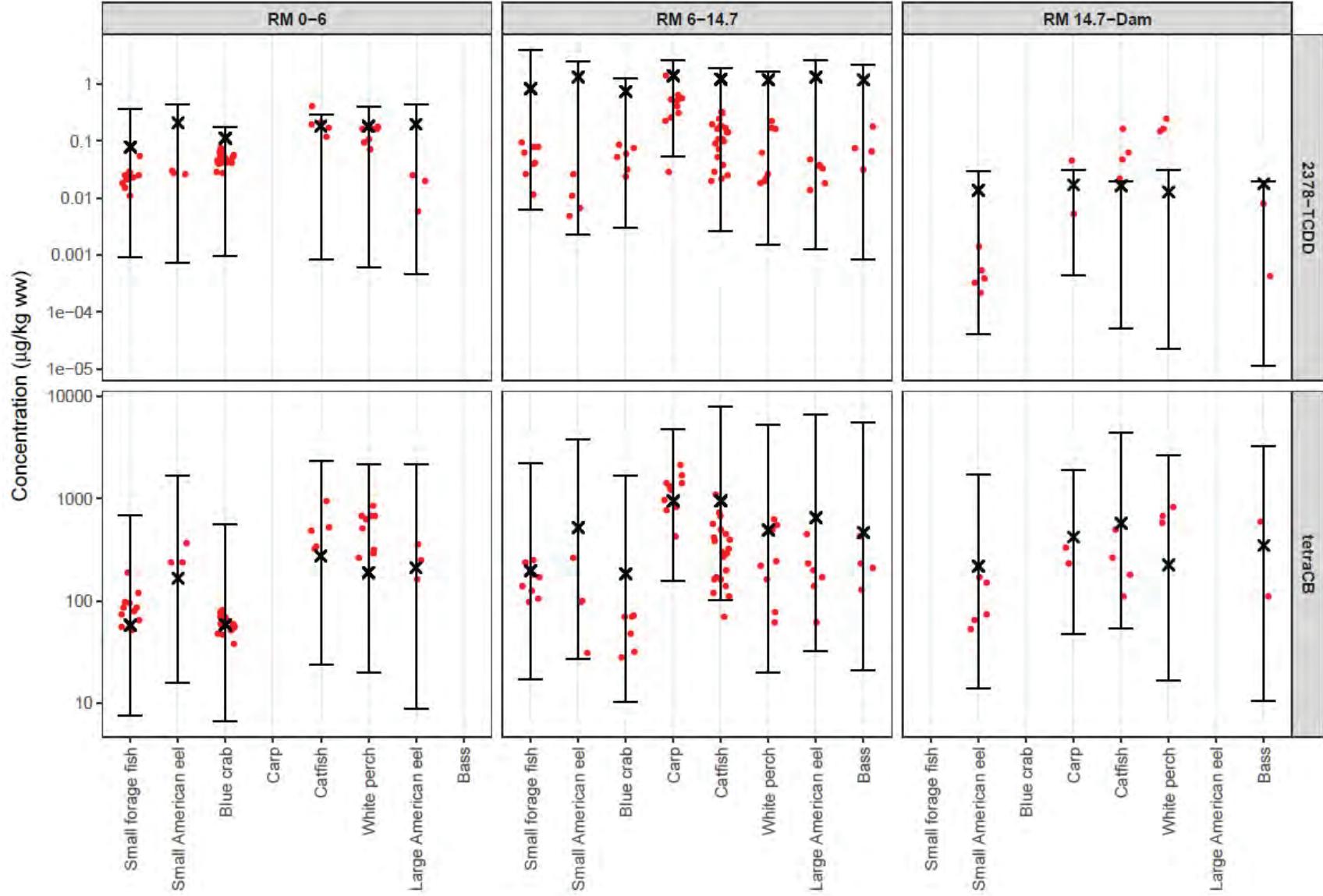


Alternative Calibrations

- Developed following possible schemes for alternative calibrations:

	K _{ow}	Temperature	Other
CAL 1	Equal (or similar) to CFT model values	Year-round average (12-13° C)	Other changes as needed to obtain best fit.
CAL 2	Equal (or similar) to CFT model values	Warm-season average (17° C)	Other changes as needed to obtain best fit.
CAL 3	Calibrate to best fit using lower K _{ow} value.	Calibrated to obtain best fit.	Other changes as needed to obtain best fit.

Range-Finding Evaluation



Calibration 1

- Key notes:
 - K_{OW} = values from CFT model
 - Temperature = annual average (12-13° C)
- Parameter changes:

Initial model calibration, with the following revisions:

	<u>TCDD</u>	<u>Tetra</u>	<u>HpCDF</u>			
K_{OW} = same as CFT model	6.65	6	8.67			
E_D =	0.15	0.35	0.03			
	<u>inverts</u>	<u>small fish</u>	<u>crab</u>	<u>eel</u>	<u>carp</u>	<u>other fish</u>
K_M for TCDD =	0.06	0.02	0.01	0.04	0.003	0.006
K_M for TetraCB =	0	0	0.008	0.005	0	0
K_M for HpCDF =	0.15	0.07	0.02	0.036	0.036	0.036

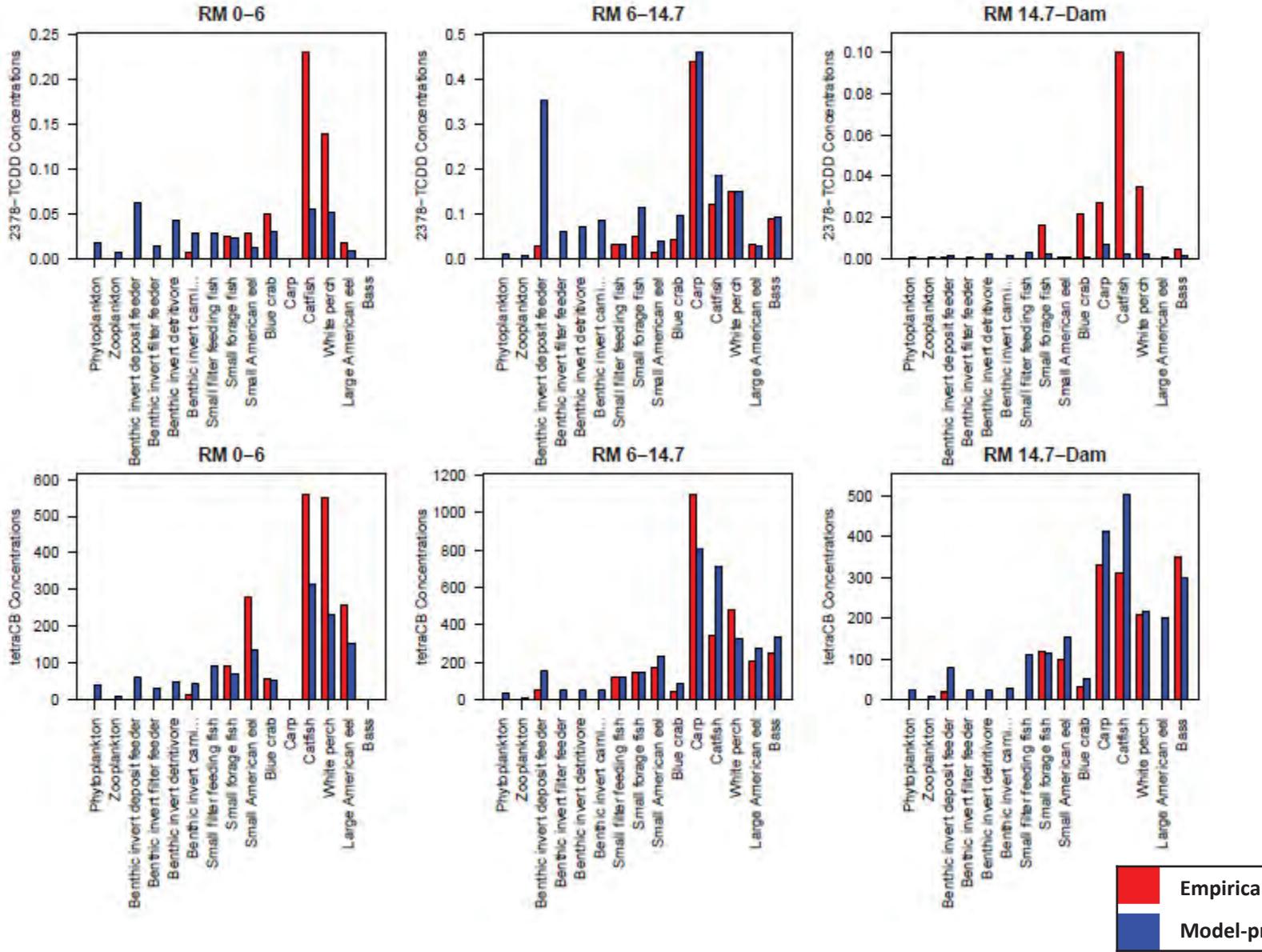
Water temperature = 12-13°C

DEP diet for RM 0-6 = increased sediment to 70% to match other areas
(to reduce influence of Macoma on selected diet)

Calibration 1 Results – SPAFs

Species	2378-TCDD			TetraCB			1234678-HpCDF		
	RM 0-6	RM 6- 14.7	RM 14.7- Dam	RM 0-6	RM 6- 14.7	RM 14.7- Dam	RM 0-6	RM 6- 14.7	RM 14.7- Dam
DEP		12.2	3.1		2.8	3.7		6.4	1.3
FF									
DET									
C/O	4.5			2.9			2.7		
Small filter feeding fish		1.1			-1.0			-1.0	
Small forage fish	-1.1	2.3	-7.6	-1.3	-1.0	-1.0	2.3	-1.1	-1.6
Small American eel	-2.4	2.8	-1.3	-2.1	1.3	1.5	-1.6	1.8	-1.1
Blue crab	-1.7	2.3	-25.7	-1.1	1.9	1.5	-1.9	1.2	-2.0
Carp		1.0	-4.2		-1.4	1.2		-1.3	1.1
Catfish	-4.2	1.5	-39.4	-1.8	2.1	1.6	-2.0	3.1	1.4
White perch	-2.7	-1.0	-14.7	-2.4	-1.5	1.0	1.2	1.8	2.1
Large American eel	-2.0	-1.1		-1.7	1.3		-1.2	1.1	
Bass		1.0	-3.2		1.4	-1.2		-1.2	-3.8
Average (all)	2.4	1.6	13.7	1.7	1.4	1.3	1.7	1.5	1.8
Average (priority)	1.8			1.5			1.6		

Calibration 1 Results - Plots



Empirical data
Model-predicted

Calibration 2

- Key notes:
 - KOW = values from CFT model
 - Temperature = warm-season average (17° C)
- Parameter changes:

Initial model calibration, with the following revisions:

	TCDD	Tetra	HpCDF			
K _{ow} = same as CFT model	6.65	6	8.67			
E _D =	0.12	0.3	0.02			
	inverts	s-fish	crab	eel	carp	other fish
K _M for TCDD =	0.06	0.02	0.01	0.04	0.003	0.006
K _M for TetraCB =	0	0	0.008	0.002	0	0
K _M for HpCDF =	0.15	0.07	0.015	0.03	0.03	0.03

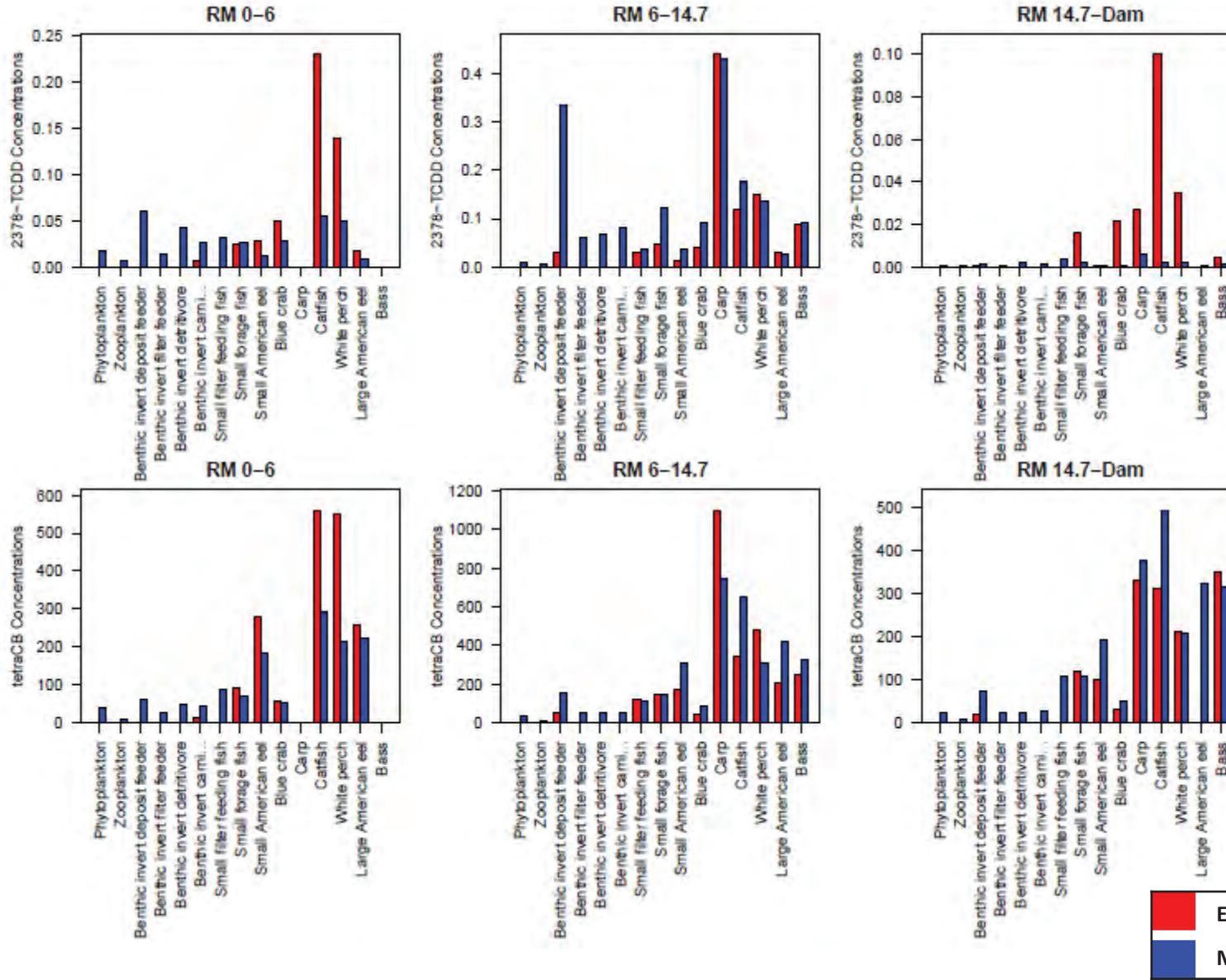
water temperature = 17° C for all areas

DEP diet for RM 0-6 = increased sediment to 70% to match other areas
(to reduce influence of Macoma on selected diet)

Calibration 2 Results – SPAFs

Species	2378-TCDD			TetraCB			1234678-HpCDF		
	RM 0-6	RM 6- 14.7	RM 14.7- Dam	RM 0-6	RM 6- 14.7	RM 14.7- Dam	RM 0-6	RM 6- 14.7	RM 14.7- Dam
DEP		11.6	3.0		2.8	3.6		5.3	1.1
FF									
DET									
C/O	4.4			2.9			2.3		
Small filter feeding fish		1.2			-1.1			-1.2	
Small forage fish	1.0	2.5	-6.8	-1.3	-1.0	-1.1	1.9	-1.4	-1.9
Small American eel	-2.4	2.8	-1.3	-1.5	1.8	1.9	-1.6	1.7	-1.2
Blue crab	-1.7	2.2	-27.2	-1.1	1.8	1.6	-1.9	1.2	-2.1
Carp		-1.0	-4.5		-1.5	1.1		-1.3	1.0
Catfish	-4.2	1.5	-41.1	-1.9	1.9	1.6	-2.0	3.1	1.4
White perch	-2.8	-1.1	-16.0	-2.5	-1.6	-1.0	1.1	1.7	1.9
Large American eel	-1.9	-1.1		-1.2	2.0		-1.2	1.0	
Bass		1.0	-3.2		1.3	-1.1		-1.4	-4.7
Average (all)	2.3	1.6	14.3	1.6	1.6	1.4	1.6	1.6	2.0
Average (priority)		1.8			1.7			1.6	

Calibration 2 Results - Plots



Calibration 3

- Key notes:
 - K_{OW} = calibrate to best fit using lower K_{OW} value.
 - Temperature = determined as part of calibration
- Parameter changes:

Initial model calibration, with the following revisions:

	<u>TCDD</u>	<u>Tetra</u>	<u>HpCDF</u>			
K_{OW} = nominal / lower value	6	5.85	8.03			
E_D =	0.17	0.4	0.02			
	<u>inverts</u>	<u>small fish</u>	<u>crab</u>	<u>eel</u>	<u>carp</u>	<u>other fish</u>
K_M for TCDD =	0.06	0.01	0.003	0.03	0.001	0.003
K_M for TetraCB =	0	0	0.005	0.002	0	0
K_M for HpCDF =	0.2	0.06	0.02	0.036	0.036	0.036

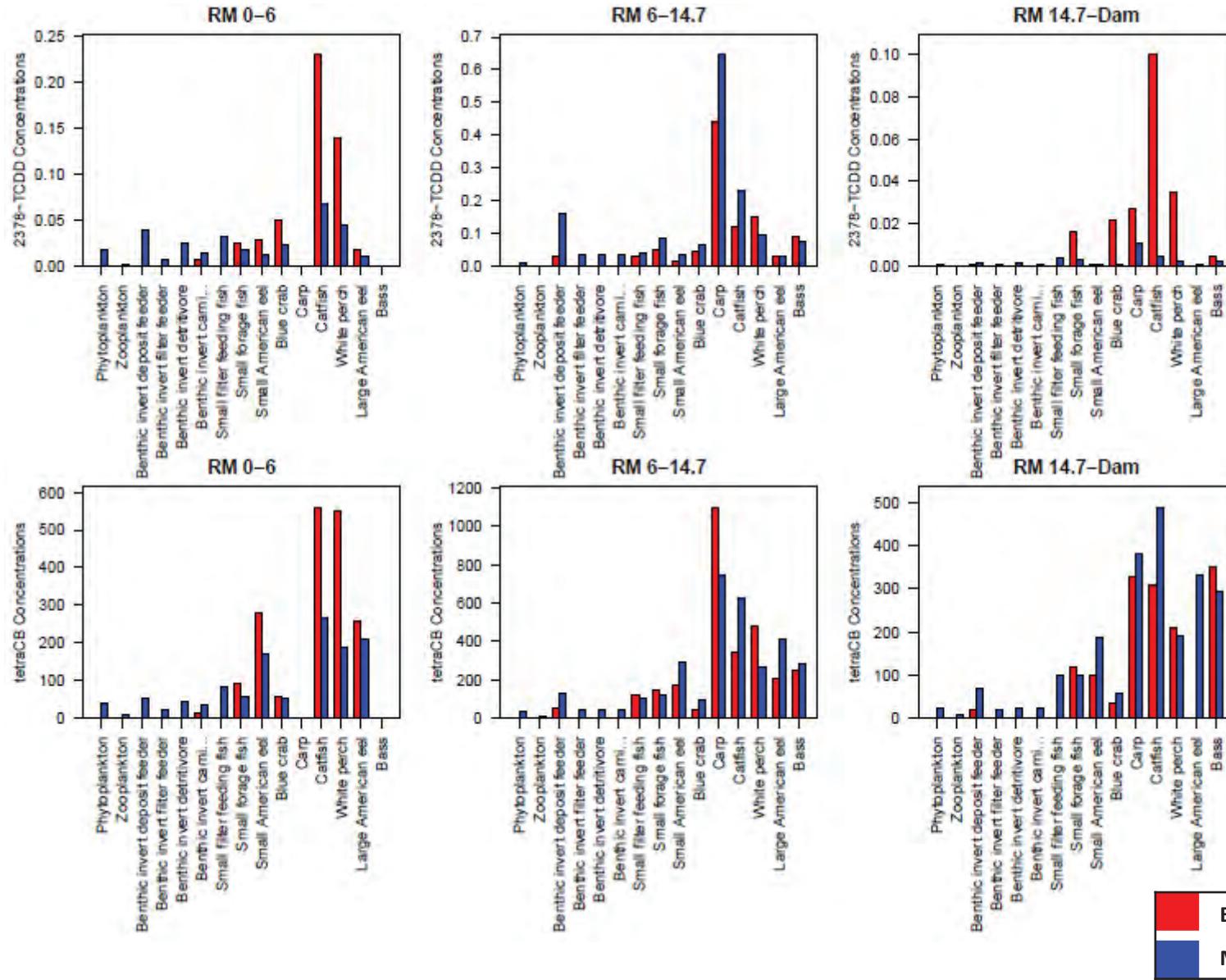
Water temperature = 15° C

DEP diet for RM 0-6 = increased sediment to 70% to match other areas
(to reduce influence of Macoma on selected diet)

Calibration 3 Results – SPAFs

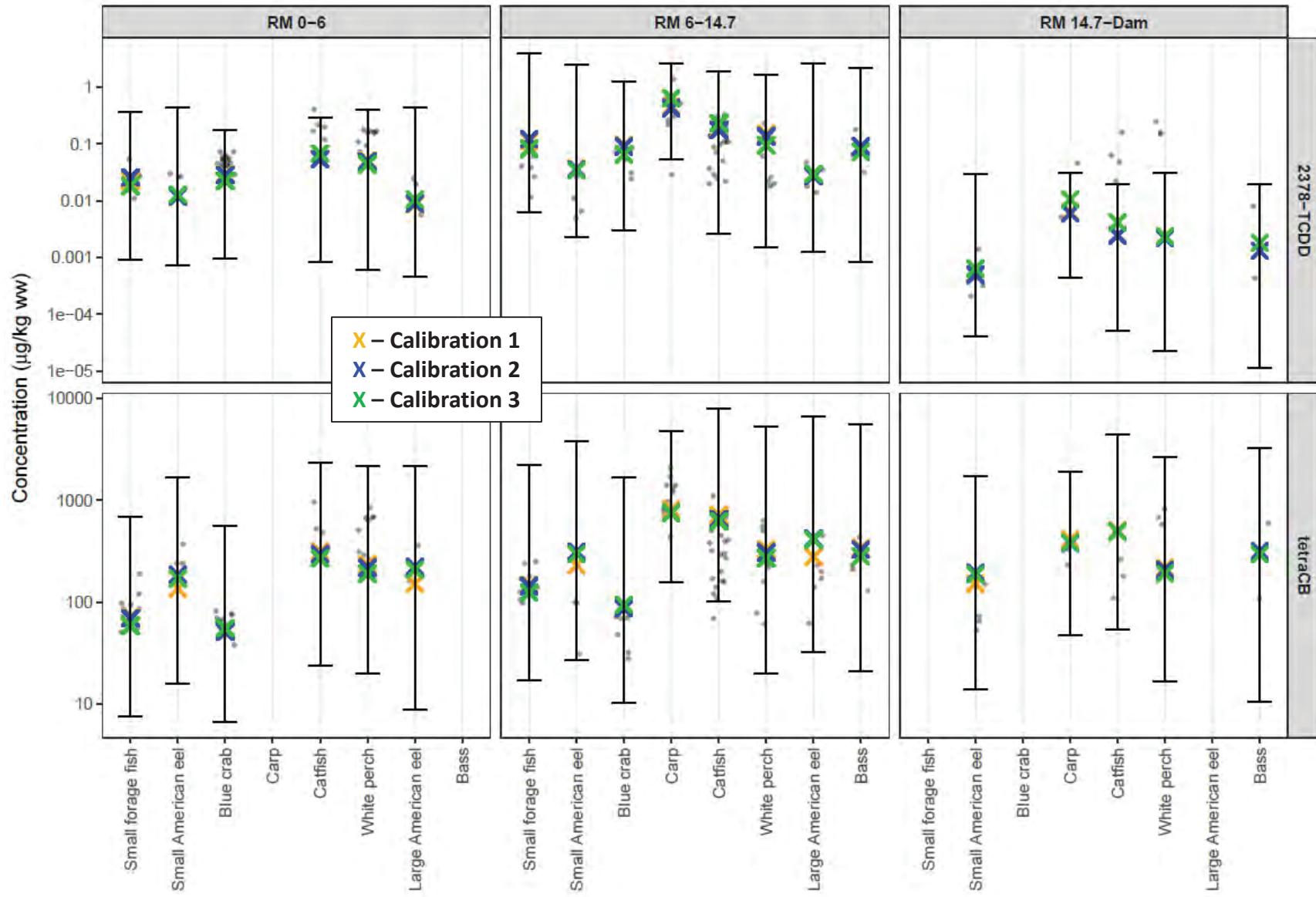
Species	2378-TCDD			TetraCB			1234678-HpCDF		
	RM 0-6	RM 6- 14.7	RM 14.7- Dam	RM 0-6	RM 6- 14.7	RM 14.7- Dam	RM 0-6	RM 6- 14.7	RM 14.7- Dam
DEP		5.5	2.7		2.5	3.3		3.6	-1.3
FF									
DET									
C/O	2.2			2.4			1.5		
Small filter feeding fish		1.3			-1.1			-1.2	
Small forage fish	-1.4	1.7	-5.8	-1.6	-1.2	-1.2	1.9	-1.4	-1.9
Small American eel	-2.2	2.6	-1.0	-1.6	1.7	1.9	-2.4	1.1	-1.7
Blue crab	-2.2	1.6	-27.1	-1.1	2.0	1.8	-3.1	-1.4	-3.4
Carp		1.5	-2.6		-1.5	1.2		-1.8	-1.3
Catfish	-3.4	1.9	-24.1	-2.1	1.8	1.6	-2.7	2.2	-1.0
White perch	-3.2	-1.6	-15.0	-2.9	-1.8	-1.1	-1.4	1.1	1.4
Large American eel	-1.6	-1.0		-1.2	1.9		-1.8	-1.4	
Bass		-1.2	-2.3		1.1	-1.2		-2.1	-7.5
Average (all)	2.3	1.6	11.1	1.8	1.6	1.4	2.2	1.5	2.6
Average (priority)	1.9			1.7			1.7		

Calibration 3 Results – Plots



Empirical data
Model-predicted

Possible Range and Calibrated Values

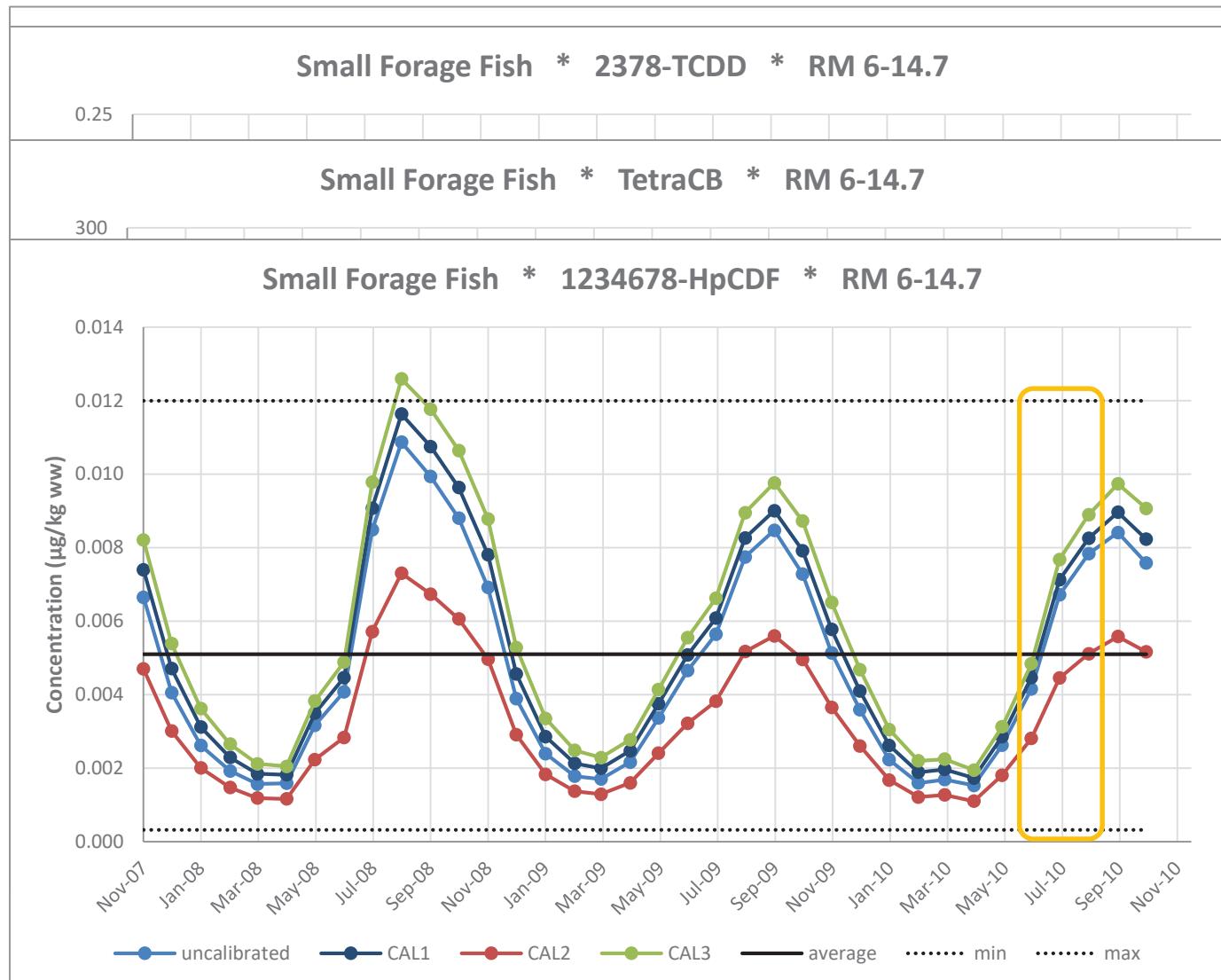


CALIBRATION REVIEW USING DYNAMIC MODEL

Key Questions to Consider

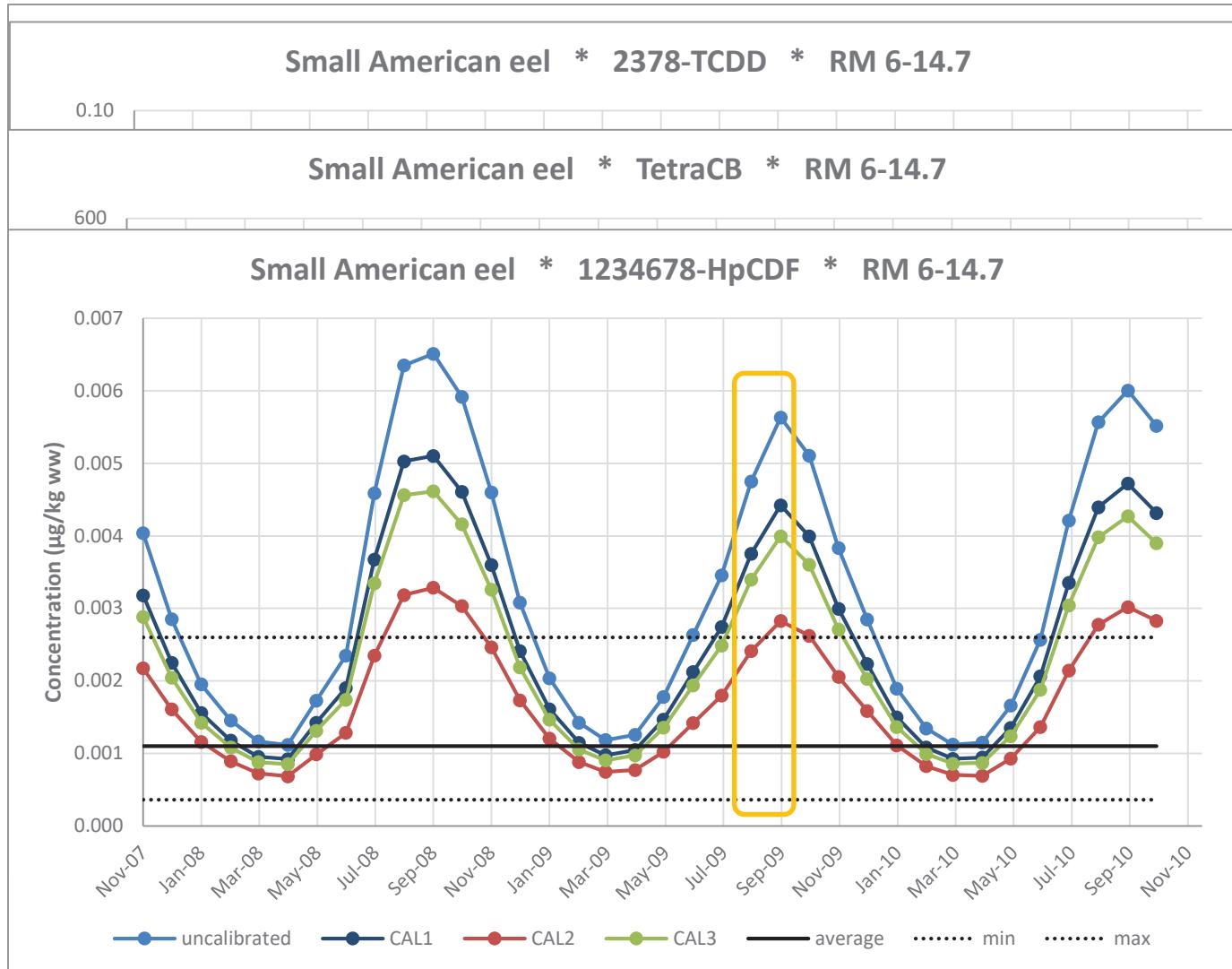
- Are seasonal fluctuations to extent shown realistic?
 - If not, what to do about this?
- How do steady state and dynamic model compare?
- How does dynamic model compare with empirical data (average and range)?

Small Forage Fish (RM 6-14.7)



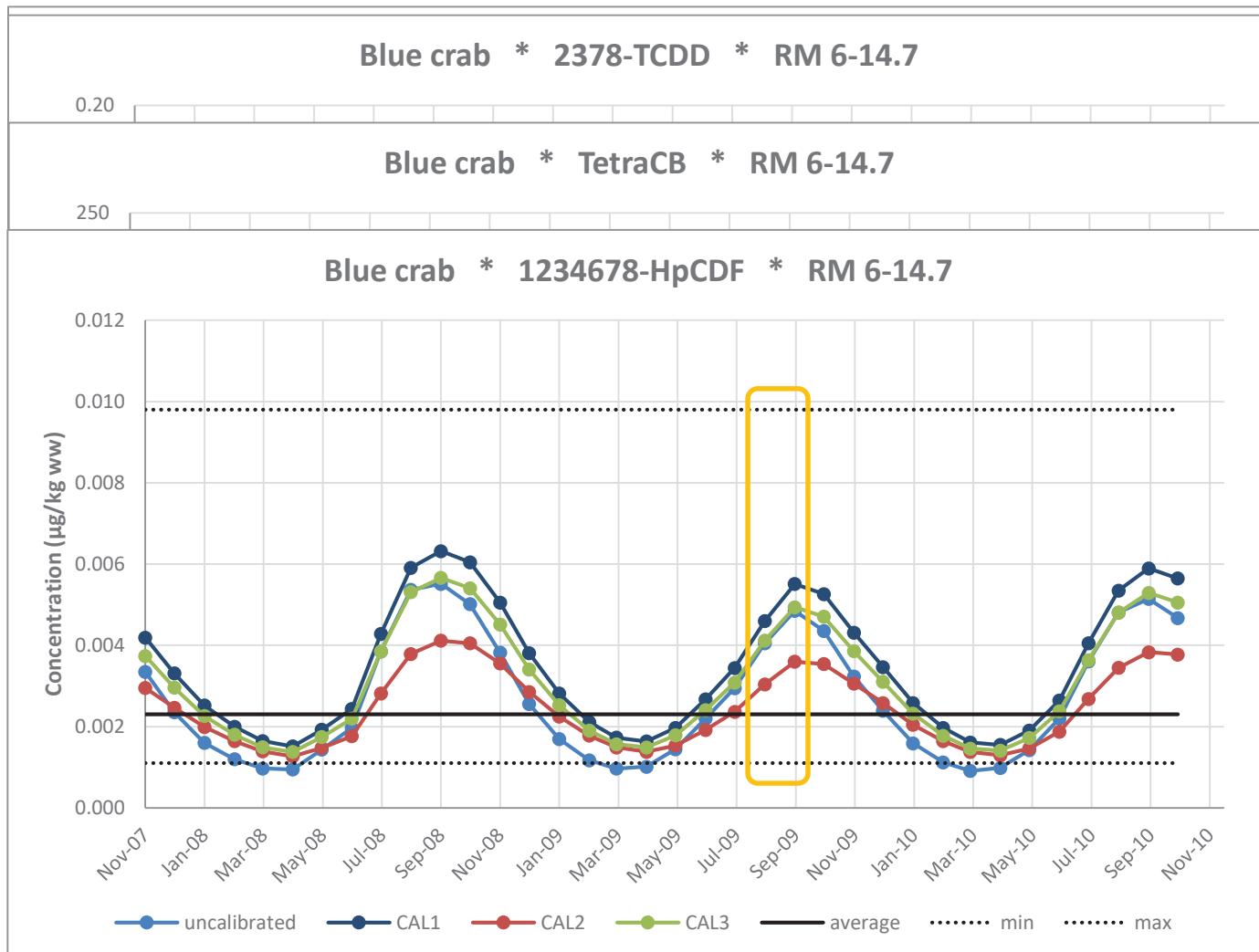
SPAFs		
2378-TCDD		
uncalibrated	17.3	
CAL1	2.3	
CAL2	2.5	
CAL3	1.7	
TetraCB		
uncalibrated	1.3	
CAL1	-1.0	
CAL2	-1.0	
CAL3	-1.2	
1234678-HpCDF		
uncalibrated	-1.3	
CAL1	-1.1	
CAL2	-1.4	
CAL3	-1.4	

Small American eel (RM 6-14.7)



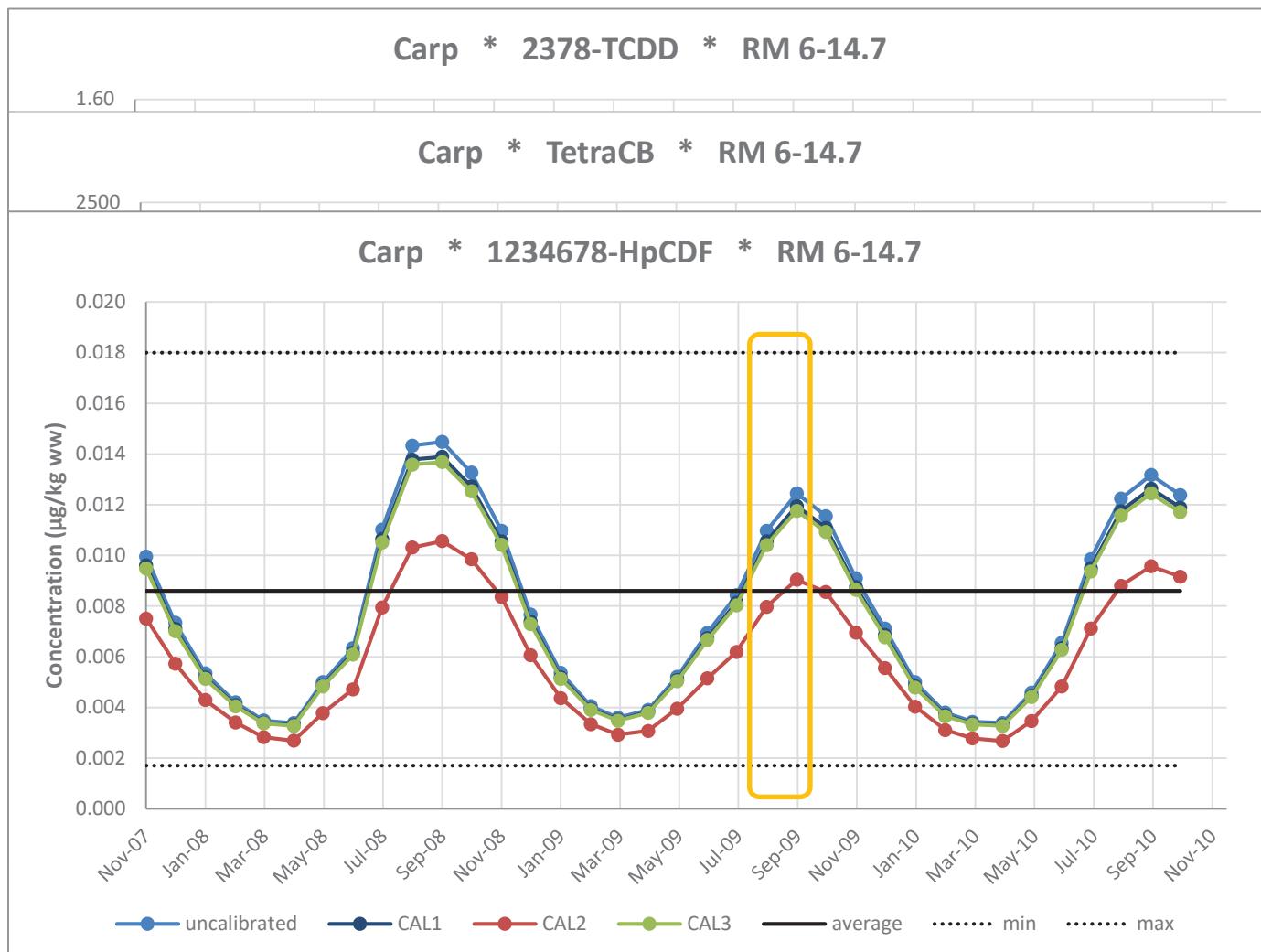
SPAFs	
2378-TCDD	
uncalibrated	103.1
CAL1	2.8
CAL2	2.8
CAL3	2.6
TetraCB	
uncalibrated	3.1
CAL1	1.3
CAL2	1.8
CAL3	1.7
1234678-HpCDF	
uncalibrated	2.1
CAL1	1.8
CAL2	1.7
CAL3	1.1

Blue crab (RM 6-14.7)



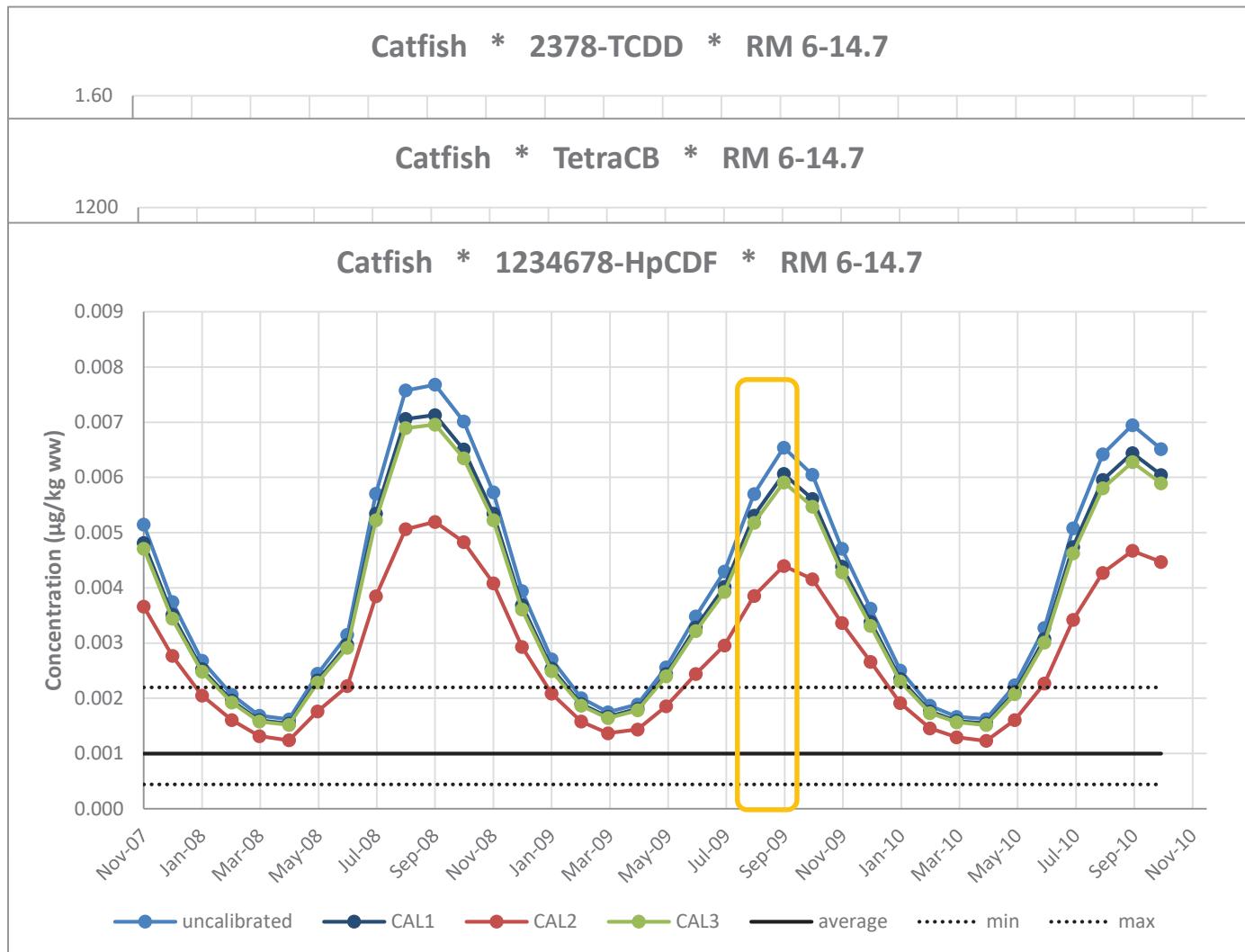
SPAFs		
2378-TCDD		
uncalibrated	17.8	
CAL1	2.3	
CAL2	2.2	
CAL3	1.6	
TetraCB		
uncalibrated	3.9	
CAL1	1.9	
CAL2	1.8	
CAL3	2.0	
1234678-HpCDF		
uncalibrated	-1.2	
CAL1	1.2	
CAL2	1.2	
CAL3	-1.4	

Carp (RM 6-14.7)



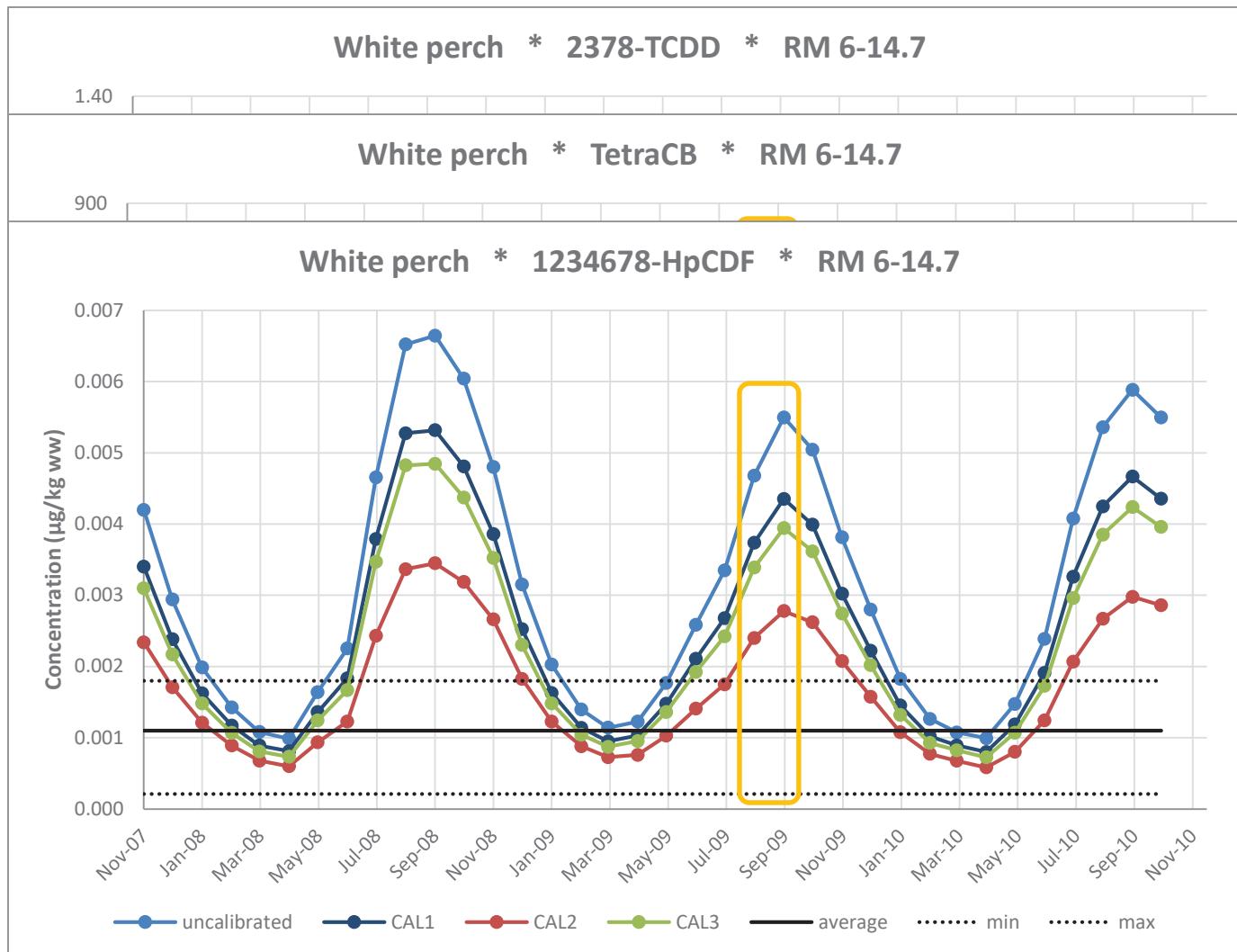
SPAFs		
2378-TCDD		
uncalibrated	3.2	
CAL1	1.0	
CAL2	-1.0	
CAL3	1.5	
TetraCB		
uncalibrated	-1.2	
CAL1	-1.4	
CAL2	-1.5	
CAL3	-1.5	
1234678-HpCDF		
uncalibrated	-1.3	
CAL1	-1.3	
CAL2	-1.3	
CAL3	-1.8	

Catfish (RM 6-14.7)



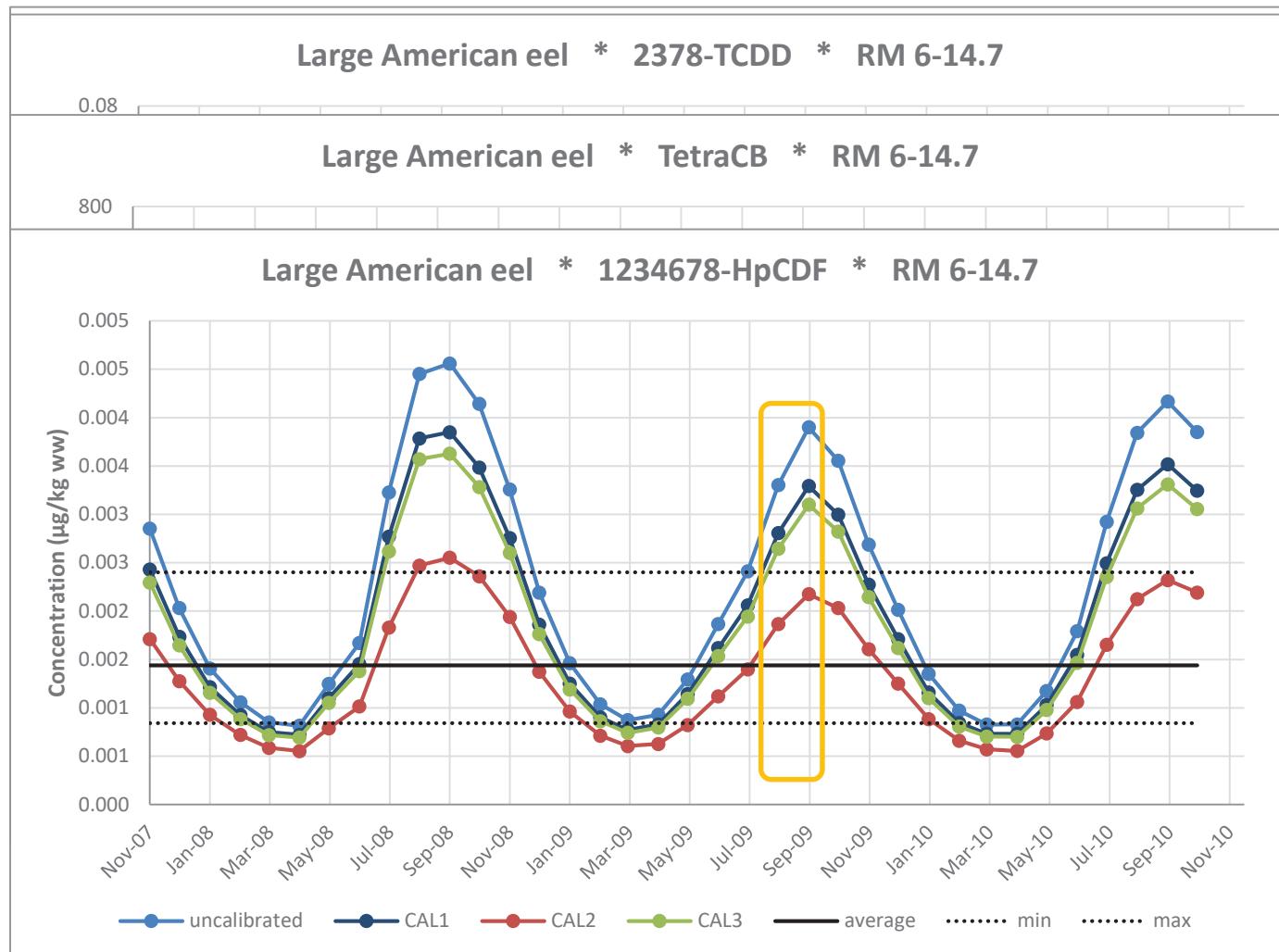
SPAFs	
2378-TCDD	
uncalibrated	10.3
CAL1	1.5
CAL2	1.5
CAL3	1.9
TetraCB	
uncalibrated	2.8
CAL1	2.1
CAL2	1.9
CAL3	1.8
1234678-HpCDF	
uncalibrated	3.3
CAL1	3.1
CAL2	3.1
CAL3	2.2

White Perch (RM 6-14.7)



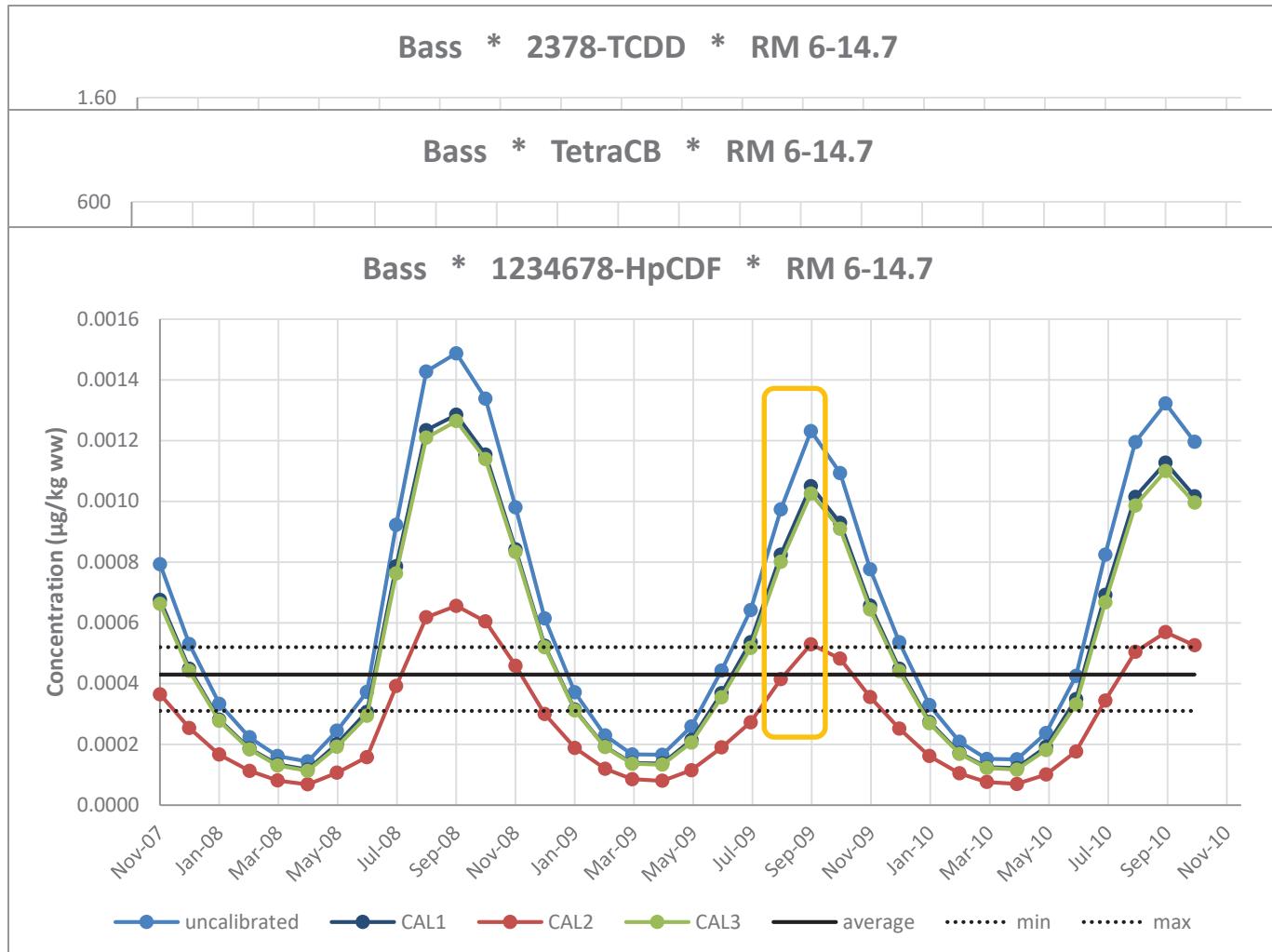
SPAFs		
2378-TCDD		
uncalibrated	7.9	
CAL1	-1.0	
CAL2	-1.1	
CAL3	-1.6	
TetraCB		
uncalibrated	1.0	
CAL1	-1.5	
CAL2	-1.6	
CAL3	-1.8	
1234678-HpCDF		
uncalibrated	2.1	
CAL1	1.8	
CAL2	1.7	
CAL3	1.1	

Large American Eel (RM 6-14.7)

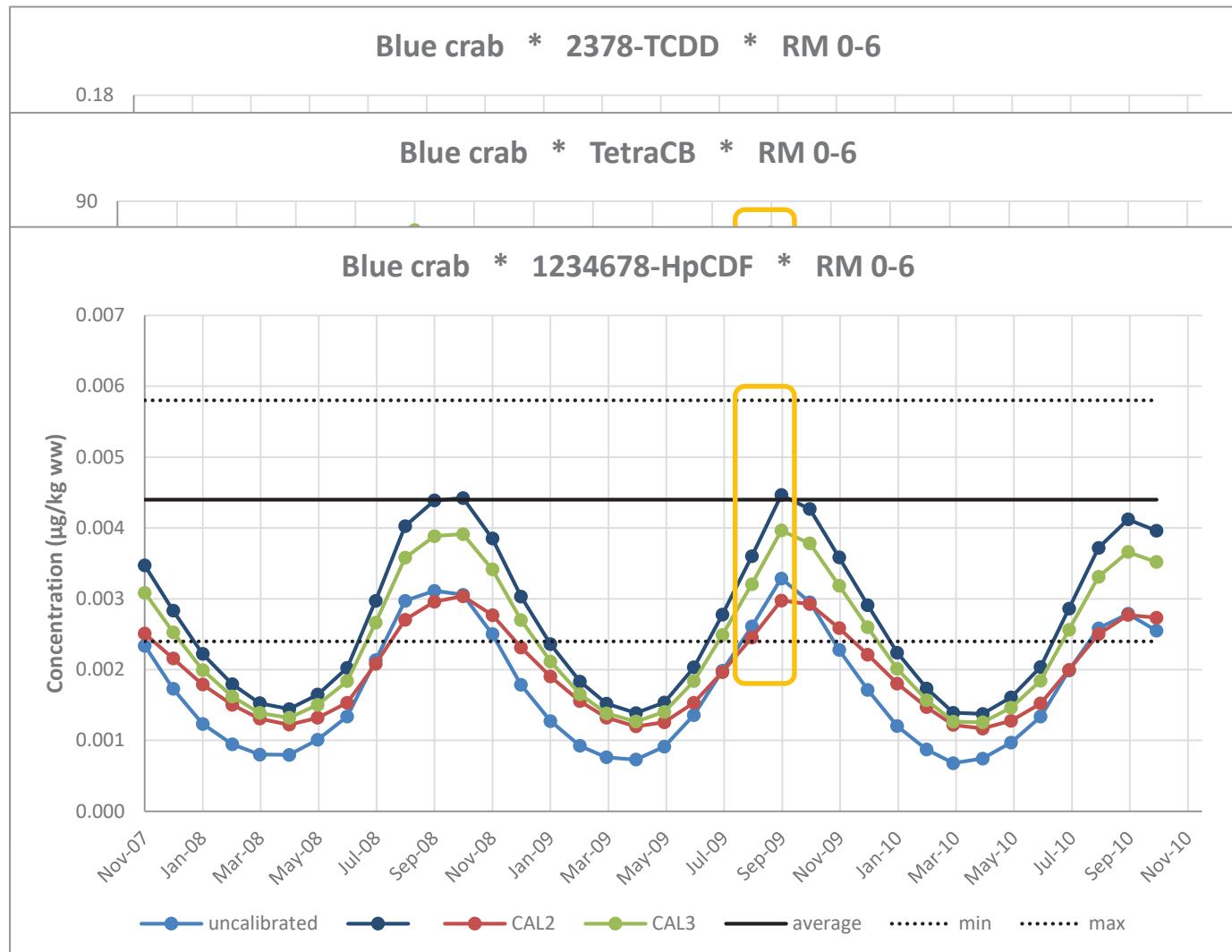


SPAFs		
2378-TCDD		
uncalibrated	43.3	
CAL1	-1.1	
CAL2	-1.1	
CAL3	-1.0	
TetraCB		
uncalibrated	3.1	
CAL1	1.3	
CAL2	2.0	
CAL3	1.9	
1234678-HpCDF		
uncalibrated	1.2	
CAL1	1.1	
CAL2	1.0	
CAL3	-1.4	

Bass (RM 6-14.7)

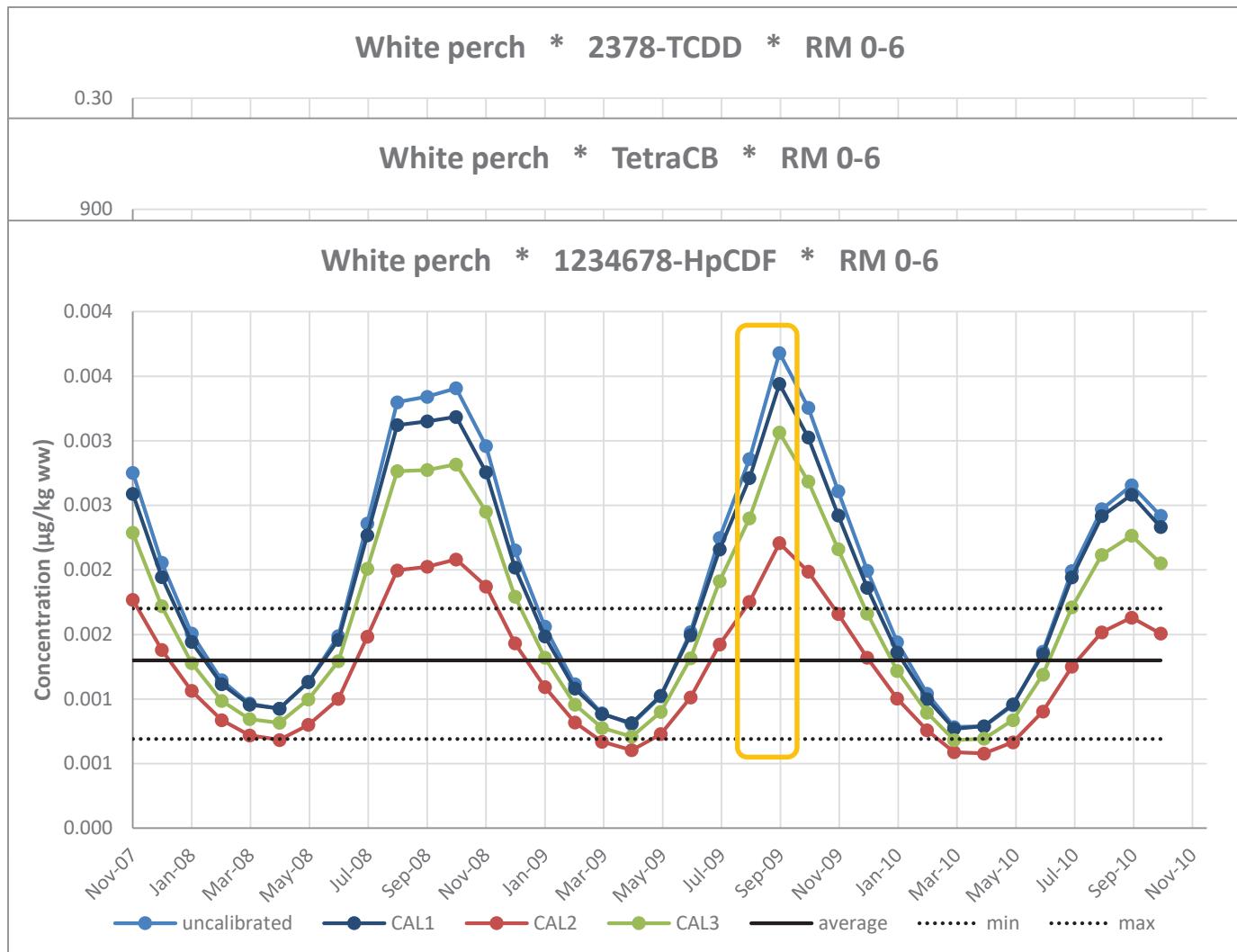


Blue Crab (RM 0-6)



SPAFs	
2378-TCDD	
uncalibrated	2.3
CAL1	2.3
CAL2	2.2
CAL3	1.6
TetraCB	
uncalibrated	-1.0
CAL1	1.9
CAL2	1.8
CAL3	2.0
1234678-HpCDF	
uncalibrated	-3.1
CAL1	1.2
CAL2	1.2
CAL3	-1.4

White Perch (RM 0-6)



SPAFs		
2378-TCDD		
uncalibrated	1.3	
CAL1	-1.0	
CAL2	-1.1	
CAL3	-1.6	
TetraCB		
uncalibrated	-2.9	
CAL1	-1.5	
CAL2	-1.6	
CAL3	-1.8	
1234678-HpCDF		
uncalibrated	1.2	
CAL1	1.8	
CAL2	1.7	
CAL3	1.1	



NEXT STEPS

Next Steps

- Feedback from EPA?
- Action items from meeting?
- Schedule dependent on resolution of calibrations options.